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* * * * * * * * * * * Welcome to STN International * * * * * * * * * * *

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NEWS 14 OCT 27 DIOGENES content streamlined
NEWS 15 OCT 27 EPFULL enhanced with additional content
NEWS 16 NOV 14 CA/CAplus - Expanded coverage of German academic research

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

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FILE 'HOME' ENTERED AT 15:31:15 ON 14 NOV 2005

=> file reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

| | |
|---------------------|------------------|
| SINCE FILE
ENTRY | TOTAL
SESSION |
| 0.21 | 0.21 |

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STRUCTURE FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0
DICTIONARY FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
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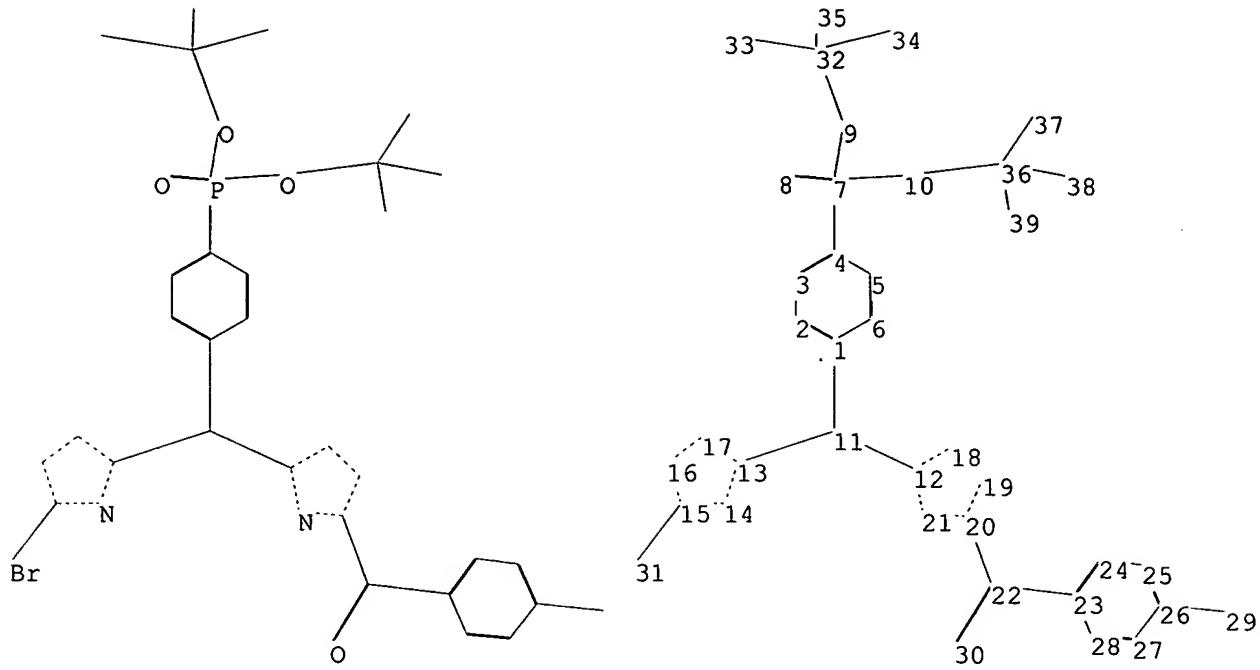
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10698255s.str



```

chain nodes :
7 8 9 10 11 22 29 30 31 32, 33 34 35 36 37 38 39
ring nodes :
1 2 3 4 5 6 12 13 14 15 16 17 18 19 20 21 23 24 25 26 27 28
chain bonds :
1-11 4-7 7-8 7-9 7-10 9-32 10-36 11-12 11-13 15-31 20-22 22-23 22-30
26-29 32-33 32-34 32-35 36-37 36-38 36-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-21 13-14 13-17 14-15 15-16 16-17
18-19 19-20 20-21 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
7-8 7-9 7-10 9-32 10-36 12-18 12-21 13-14 13-17 14-15 15-16 16-17 18-19
19-20 20-21 22-30
exact bonds :
1-11 4-7 11-12 11-13 15-31 20-22 22-23 26-29 32-33 32-34 32-35 36-37
36-38 36-39
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 23-24 23-28 24-25 25-26 26-27 27-28

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:CLASS

```

```

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11
SAMPLE SEARCH INITIATED 15:31:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 15:31:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L3 1 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
                           ENTRY SESSION
FULL ESTIMATED COST           161.33 161.54

FILE 'CAPLUS' ENTERED AT 15:31:48 ON 14 NOV 2005
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FILE COVERS 1907 - 14 Nov 2005 VOL 143 ISS 21
FILE LAST UPDATED: 13 Nov 2005 (20051113/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 13
L4 2 L3

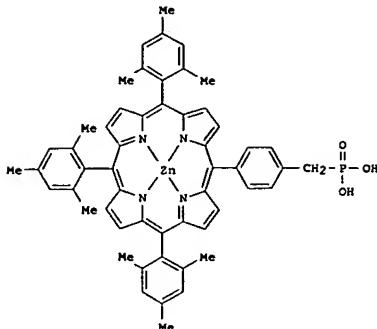
=> d ibib abs hitstr tot

```

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2005:394876 CAPLUS
 DOCUMENT NUMBER: 142:440857
 TITLE: Synthesis of phosphono-substituted porphyrin compounds
 INVENTOR(S): Lindsey, Jonathan S.; Loewe, Robert S.; Muthukumaran, Kannan; Ambroise, Arounaguiry
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 29 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

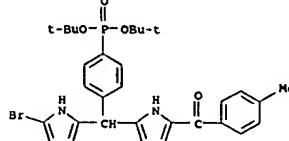
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| US 2005096465 | A1 | 20050505 | US 2003-698255 | 20031031 |
| PRIORITY APPLN. INFO.: | | | US 2003-698255 | 20031031 |

GI



AB A method is described for making phosphono-substituted dipyrromethane derivs. comprising reacting an aldehyde or acetal having at least one phosphono group with pyrrole to produce a phosphono-substituted dipyrromethane. The phosphono substituent is selected from the group consisting of dialkyl phosphono, diaryl phosphono, and dialkylaryl phosphono. The dipyrromethane is used to prepare phosphono-substituted chlorins and porphyrins which can potentially be attached to metal oxide surfaces. Thus, zinc 5-(4-(phosphonomethyl)phenyl)-10,15,20-

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 trimesitylporphyrin (I) was prep'd. Addnl. methods, intermediates and products are also described.
 IT 651302-30-6
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of phosphono-substituted porphyrin compds.)
 RN 651302-30-6 CAPLUS
 CN Phosphonic acid, [4-[{5-bromo-1H-pyrrol-2-yl}{5-(4-methylbenzoyl)-1H-pyrrol-2-yl}methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2003:965574 CAPLUS
 DOCUMENT NUMBER: 140:156138
 TITLE: Porphyrins Bearing Arylphosphonic Acid Tethers for Attachment to Oxide Surfaces
 AUTHOR(S): Muthukumaran, Kannan; Loewe, Robert S.; Ambroise, Arounaguiry; Tamari, Shunichi; Li, Qiliang; Mathur, Guru; Bocian, David F.; Misra, Veena; Lindsey, Jonathan S.
 CORPORATE SOURCE: Department of Chemistry and Electrical and Computer Engineering, North Carolina State University, Raleigh,
 SOURCE: NC, 27695-8204, USA
 Journal of Organic Chemistry (2004), 69(5), 1444-1452
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

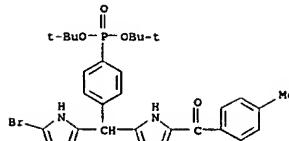
AB Synthetic mols. bearing phosphonic acid groups can be readily attached to oxide surfaces. As part of a program in mol.-based information storage, the authors have developed routes for the synthesis of diverse

porphyrinic compds. bearing phenylphosphonic acid tethers. The routes enable (1) incorporation of masked phosphonic acid groups in precursors for use in the rational synthesis of porphyrinic compds. and (2) derivatization of porphyrins with masked phosphonic acid groups. The precursors include dipyrromethanes, monoacyldipyrromethanes, and diacyldipyrromethanes. The tert-Bu group was used to mask the dihydroxyphosphoryl substituent. The di-tert-butylphosphoryl unit is stable to the range of conditions employed in syntheses of porphyrins and multiporphyrin arrays yet can be deprotected under mild conditions (TMS-Cl/TEA or TMS-Br/TEA in refluxing CHCl₃) that do not cause demetalation of Zn or Mg porphyrins. The porphyrinic compds. that were prepared include (1) A3B-, trans-A2B2-, and ABCD-porphyrins that bear a single phenylphosphonic acid group, (2) a trans-A2B2-porphyrin bearing two phenylphosphonic acid groups, (3) a chlorin that bears a single phenylphosphonic acid group, and (4) a porphyrin dyad bearing a single phenylphosphonic acid group. For selected

porphyrin-phosphonic acids, the electrochem characteristics were studied for mols. tethered to SiO₂ surfaces grown on doped Si. The voltammetric behavior indicates that the porphyrin-phosphonic acids form robust, elec. well-behaved monolayers on the oxide surface.

IT 651302-30-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of magnesium/zinc complexes with porphyrins having arylphosphonic acid tethers)
 RN 651302-30-6 CAPLUS
 CN Phosphonic acid, [4-[{5-bromo-1H-pyrrol-2-yl}{5-(4-methylbenzoyl)-1H-pyrrol-2-yl}methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

| | | | |
|--|------------------|---------------|--|
| => file reg | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 10.33 | 171.87 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | -1.46 | -1.46 | |

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STRUCTURE FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0
 DICTIONARY FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0

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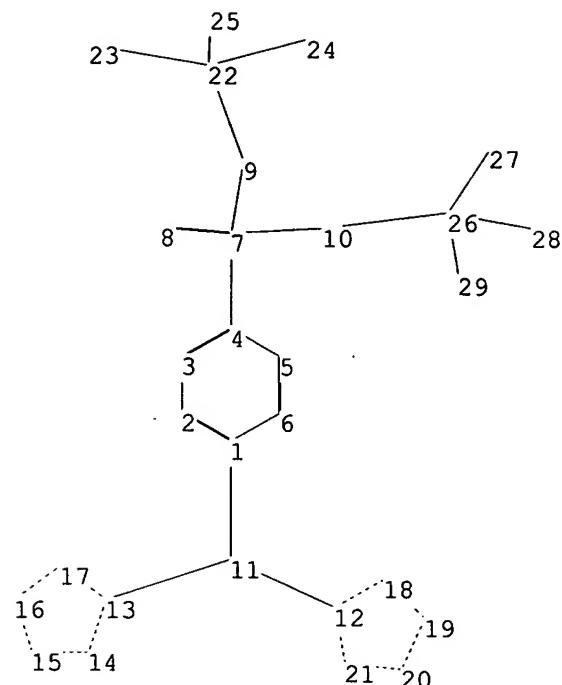
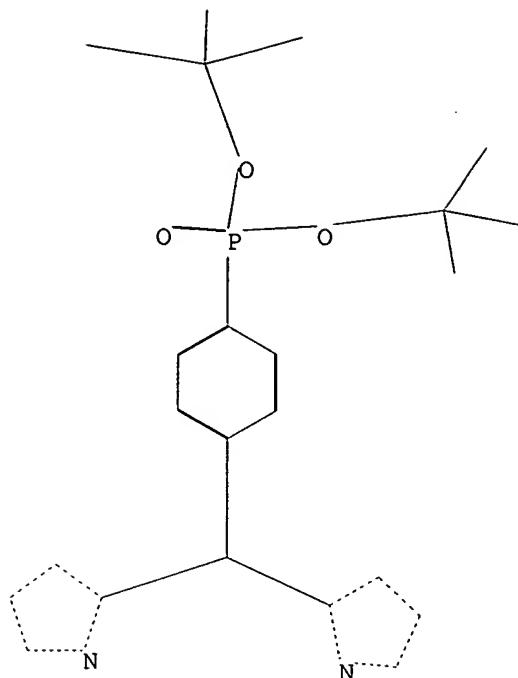
 *
 * The CA roles and document type information have been removed from *
 * the IDE default display format and the ED field has been added, *
 * effective March 20, 2005. A new display format, IDERL, is now *
 * available and contains the CA role and document type information. *
 *

Structure search iteration limits have been increased. See HELP SLIMITS . for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>
 Uploading C:\Program Files\Stnexp\Queries\10698255.str



chain nodes :

7 8 9 10 11 22 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17 18 19 20 21

chain bonds :

1-11 4-7 7-8 7-9 7-10 9-22 10-26 11-12 11-13 22-23 22-24 22-25 26-27
26-28 26-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-21 13-14 13-17 14-15 15-16 16-17
18-19 19-20 20-21

exact/norm bonds :

7-8 7-9 7-10 9-22 10-26 12-18 12-21 13-14 13-17 14-15 15-16 16-17 18-19
19-20 20-21

exact bonds :

1-11 4-7 11-12 11-13 22-23 22-24 22-25 26-27 26-28 26-29

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS

L5 STRUCTURE UPLOADED

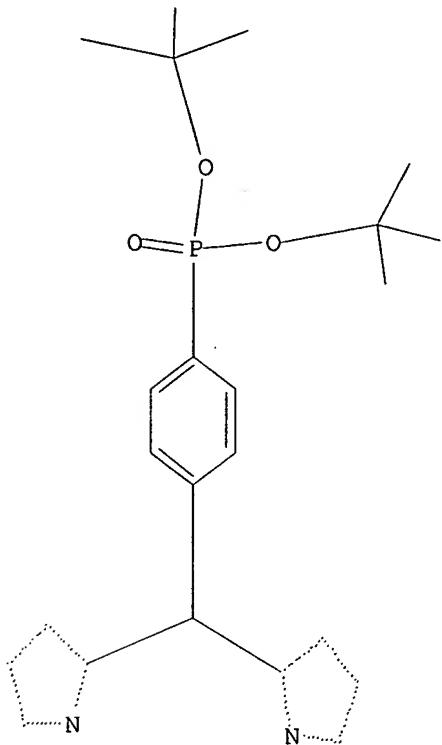
=> dd

DD IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15
SAMPLE SEARCH INITIATED 15:33:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s 15 full
FULL SEARCH INITIATED 15:33:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L7 4 SEA SSS FUL L5

| | | |
|--|------------------|---------------|
| => file caplus | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 161.76 | 333.63 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.46 |

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FILE COVERS 1907 - 14 Nov 2005 VOL 143 ISS 21
FILE LAST UPDATED: 13 Nov 2005 (20051113/ED)

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<http://www.cas.org/infopolicy.html>

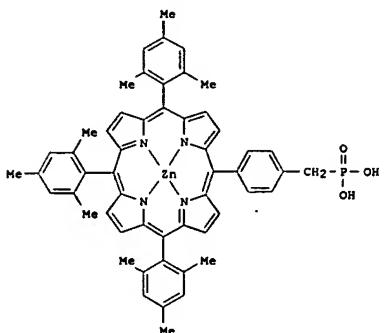
=> s 17
L8 2 L7

=> d ibib abs hitstr tot

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2005:394876 CAPLUS
 DOCUMENT NUMBER: 142:440857
 TITLE: Synthesis of phosphono-substituted porphyrin compounds
 INVENTOR(S): Lindsey, Jonathan S.; Loewe, Robert S.; Muthukumaran, Kannan; Ambroise, Arounaguiry USA
 PATENT ASSIGNEE(S): U.S. Pat. Appl. Publ., 29 pp.
 SOURCE: CODEN: USXKCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| US 2005096465 | A1 | 20050505 | US 2003-698255 | 20031031 |
| PRIORITY APPLN. INFO.: | | | US 2003-698255 | 20031031 |

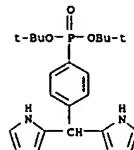
GI



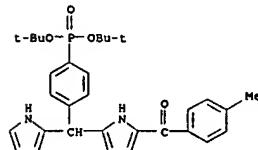
I

AB A method is described for making phosphono-substituted dipyrromethane derivs. comprising reacting an aldehyde or acetal having at least one phosphono group with pyrrole to produce a phosphono-substituted dipyrromethane. The phosphono substituent is selected from the group consisting of dialkyl phosphono, diaryl phosphono, and dialkylaryl phosphono. The dipyrromethane is used to prepare phosphono-substituted chlorins and porphyrins which can potentially be attached to metal oxide surfaces. Thus, zinc 5-[4-(phosphonomethyl)phenyl]-10,15,20-

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 trimesitylporphyrin (I) was prep'd. Addnl. methods, intermediates and products are also described.
 IT 651301-78-9 651301-87-0P 651301-88-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of phosphono-substituted porphyrin compds.)
 RN 651301-78-9 CAPLUS
 CN Phosphonic acid, [4-(di-1H-pyrrol-2-ylmethyl)phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

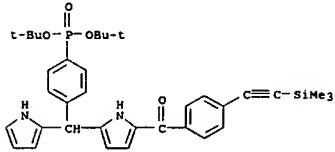


RN 651301-87-0 CAPLUS
 CN Phosphonic acid, [4-[(5-(4-methylbenzoyl)-1H-pyrrol-2-yl)-1H-pyrrol-2-ylmethyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

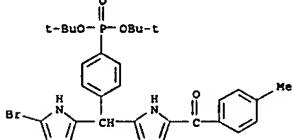


RN 651301-88-1 CAPLUS
 CN Phosphonic acid, [4-[1H-pyrrol-2-yl[5-[(4-[(trimethylsilyl)ethynyl]benzoyl)-1H-pyrrol-2-yl]methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT 651302-30-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of phosphono-substituted porphyrin compds.)
 RN 651302-30-6 CAPLUS
 CN Phosphonic acid, [4-[(5-bromo-1H-pyrrol-2-yl)(5-(4-methylbenzoyl)-1H-pyrrol-2-yl)methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2003:965574 CAPLUS
 140:156138
 DOCUMENT NUMBER:
 Porphyrins Bearing Arylphosphonic Acid Tethers for
 Attachment to Oxide Surfaces
 TITLE:
 AUTHOR(S): Muthukumaran, Kannan; Loewe, Robert S.; Ambroise,
 Arounaguiry; Tamaru, Shunichi; Li, Qiliang; Mathur,
 Guru; Bocian, David F.; Misra, Veena; Lindsey,
 Jonathan S.

CORPORATE SOURCE: Departments of Chemistry and Electrical and Computer
 Engineering, North Carolina State University, Raleigh,

RALEIGH,
 SOURCE: NC 27695-8204, USA
 Journal of Organic Chemistry (2004), 69(5), 1444-1452
 PUBLISHER: CODEN: JOCEAH; ISSN: 0022-3263
 American Chemical Society

DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Synthetic mols. bearing phosphonic acid groups can be readily attached to
 oxide surfaces. As part of a program in mol.-based information storage,
 the authors have developed routes for the synthesis of diverse
 porphyrinic

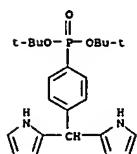
compds. bearing phenylphosphonic acid tethers. The routes enable (1) incorporation of masked phosphonic acid groups in precursors for use in the rational synthesis of porphyrinic compds. and (2) derivatization of porphyrins with masked phosphonic acid groups. The precursors include dipyrromethanes, monoacyldipyrromethanes, and diacyldipyrromethanes. The tert-Bu group was used to mask the dihydroxyphosphoryl substituent. The di-tert-butyl group is stable to the range of conditions employed in syntheses of porphyrins and multiporphyrin arrays yet can be deprotected under mild conditions (TMS-Cl/TFA or TMS-Br/TFA in refluxing CHCl3) that do not cause demetalation of Zn or Mg porphyrins. The porphyrinic compds. that were prepared include (1) A3B-, trans-A2B2C-, and trans-A2B2-porphyrin bearing two phenylphosphonic acid groups, (2) a chlorin that bears a single phenylphosphonic acid group, and (4) a porphyrin dyad bearing a single phenylphosphonic acid group. For

selected porphyrin-phosphonic acids, the electrochem. characteristics were studied for mols. tethered to SiO2 surfaces grown on doped Si. The voltammetric behavior indicates that the porphyrin-phosphonic acids form robust, elec. well-behaved monolayers on the oxide surface.

IT 651301-78-9 651301-87-0P 651301-88-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reactant for preparation of zinc/magnesium complexes
 with porphyrins having arylphosphonic acid tethers)

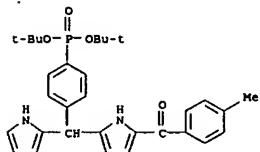
RN 651301-78-9 CAPLUS

CN Phosphonic acid, [4-(di-1H-pyrrol-2-ylmethyl)phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



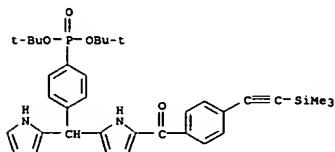
RN 651301-87-0 CAPLUS

CN Phosphonic acid, [4-[(5-(4-methylbenzoyl)-1H-pyrrol-2-yl)-1H-pyrrol-2-ylmethyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 651301-88-1 CAPLUS

CN Phosphonic acid, [4-[(5-[(4-[(trimethylsilyl)ethynyl]benzoyl)-1H-pyrrol-2-yl]methyl)phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

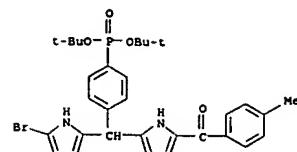


IT 651302-30-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of magnesium/zinc complexes with porphyrins having arylphosphonic acid tethers)

RN 651302-30-6 CAPLUS

CN Phosphonic acid, [4-[(5-bromo-1H-pyrrol-2-yl)[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX)

REFERENCE COUNT:
THIS48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

=> log y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 10.33 | 343.96 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -1.46 | -2.92 |

STN INTERNATIONAL LOGOFF AT 15:33:14 ON 14 NOV 2005